A MONTE CARLO APPROACH TO MEAN-SQUARE APPROXIMATION*

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* This work was supported in part by the National Aeronautics and Space Administration under Grant No. NGR-05-018-044.

ABSTRACT

An algorithm for mean-square approximation is presented. It is useful in both the case where the distribution function defining the mean is known and when it is represented solely by a finite number of samples, and may often be applied when other methods are impractical. The amount of storage required is independent of the number of sample points.

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Introduction

We consider herein the problem of finding an expression of the form $\Sigma \alpha_i \phi_i(x)$ which minimizes

$$(1) \qquad \int_{\mathcal{R}} \left[h(x) - \sum_{i=1}^{R} \alpha_i g_i(x) \right]^2 d F(x) ,$$

where $h(x)$ is a given function, $\{g_i\}$ is a set of linearly independent function, and x is a vector of dimension n. Simply, we wish to find the best mean-square approximation to $h(x)$ over the region $\mathcal{R}$.

Substantial difficulties may arise in the solution of this problem. The region R may be irregular, the vector x of high dimension, the functions $F(x)$ or $h(x)$ complex--all making the prerequisite integrations difficult. The order of approximation R may be very high, frustrating many direct methods. The probability distribution F may be unknown, defined only by a finite set of samples. Finally, $h(x)$ may be determined only by experiment upon some system (a "black box"), and hence defined at only a limited number of points [1].

The work below studies an approach which is of varying usefulness in all the above cases. We use samples of the probability distribution rather than its analytic form. The samples may result from some physical

process or be generated artificially [2,6,7]. In either case, we assume that the number of samples and their dimension is such that the problem must be solved without their storage; that is, we require that a sample be used in computation only when it is first generated and not at all thereafter. We further assume that R, the number of coefficients to be determined, is sufficiently large that the inversion of an R X R matrix is computationally infeasible. This latter assumption is related to high dimensionality: a general fifth-order polynomial in 10 variables, for example, requires 252 coefficients.

The Algorithm

The procedure proposed solves exactly the problem of minimizing

$$(2) \qquad \frac{1}{M} \sum_{j=1}^{M} \left(h(y_j) - \sum_{i=1}^{R} \alpha_i g_i(y_j) \right)^2 ,$$

where $Y = \{y_1, y_2, \ldots, y_M\}$ are sample points generated according to the distribution F. This is clearly an approximation of the problem in (1), the accuracy of the approximation increasing with M. In the case where F is unknown and Y represents our only knowledge of it, we may as well consider (2) the exact problem.

Setting the partials of (2) with respect to each coefficient equal to zero gives the necessary condition for a solution vector $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_R)$:

(3) $$A\alpha = b ,$$

where the elements of A are

(4) $$a_{ij} = \sum_{k=1}^{M} g_i (y_k)\, g_j (y_k)$$

and the components of b are

(5) $$b_i = \sum_{k=1}^{M} h (y_k)\, g_i (y_k) .$$

The conditions under which equation (3) has a unique solution will be a corollary to the work following.

If A could be inverted, the problem would be solved; the elements of A and b could be accumulated without storage of the samples by the simple iterations

(6) $$a_{ij}^{(k+1)} = a_{ij}^{(k)} + g_i (y_{k+1})\, g_j (y_{k+1}) ,$$

$$a_{ij}^{(0)} = 0 ,$$

(7) $$b_i^{(k+1)} = b_i^{(k)} + h(y_{k+1})\, g_i (y_{k+1}) ,$$

$$b_i^{(0)} = 0 ,$$

and direct solution would be possible. We have assumed, however, that A is too large to be inverted accurately.

The following algorithm yields the solution we desire:

1. The quantities $a_{ij} = a_{ij}^{(M)}$ are accumulated using (6) for $i = 1,2,\ldots,R$ and $j = i,i+1,\ldots,R$; the $b_i = b_i^{(M)}$ are accumulated using (7) for $i = 1,2,\ldots,R$.

2. Calculate

$$d_1 = a_{11}^{-\frac{1}{2}} \tag{8}$$

and store d_1 in the location where a_{11} was stored.

3. Compute

$$c_{12} = d_1 a_{12}, \tag{9}$$

and store it destructively over a_{12}.

4. For $j = 2,3,\ldots,R-1$, compute

$$d_j = \left[a_{jj} - \sum_{k=1}^{j-1} c_{kj}^2 \right]^{-\frac{1}{2}}, \tag{10}$$

$$c_{1,j+1} = d_1 a_{1,j+1}, \quad \text{and} \tag{11}$$

$$c_{i,j+1} = d_i \left[a_{i,j+1} - \sum_{k=1}^{i-1} c_{ki} c_{k,j+1} \right] \tag{12}$$

for $i = 2,3,\ldots,j$,

and finally compute d_R by (10), replacing in storage, as they are calculated, a_{jj} by d_j and a_{ij} by c_{ij}.

5. Calculate

(13) $$\beta_1 = d_1 b_1$$

(14) $$\beta_i = d_i \left[b_i - \sum_{k=1}^{i-1} c_{ki} \beta_k \right]$$

for $i = 2, 3, \ldots, R$,

storing β_i over b_i.

6. Calculate

(15) $$\alpha_R = \beta_R d_R$$

(16) $$\alpha_i = d_i (\beta_i - \sum_{j=i+1}^{R} \alpha_j c_{ij})$$

for $i = R-1, R-2, \ldots, 1$,

storing α_i over β_i.

The α_i minimize equation (2). The total amount of working storage never exceeds $\frac{R(R+3)}{2}$ words.

Derivation

To proceed we require the following notation: if $\phi(x)$ is a given function, we will write ϕ for the vector $(\phi(y_1), \phi(y_2), \ldots, \phi(y_M))$. Hence, the inner product (ϕ_1, ϕ_2) is

(17) $$(\phi_1, \phi_2) = \sum_{i=1}^{M} \phi_1(y_i) \phi_2(y_i)$$

The Gram-Schmitt orthogonalization process may be used to construct functions ortonormal over the sample points; that is, we seek a set of functions $\{\phi_1, \phi_2, \ldots, \phi_R\}$ such that

(18) $$(\phi_i, \phi_j) = \delta_{ij} ,$$

where the inner product is defined by (17). We set

(19) $$\phi_1(x) = d_1 g_1(x)$$

(20) $$\phi_i(x) = d_i[g_i(x) - c_{1i}\phi_1(x) - \cdots - c_{i-1,i}\phi_{i-1}(x)] ,$$

$$i = 2,3,\ldots,R .$$

The set $\{ g_i \}$ is a given set of linearly independent functions. We shall derive the constants d_i and c_{ij} which yield (18).

For $i < j$,

$$(\phi_i, \phi_j) = 0 = d_j(\phi_i, g_j - c_{1j}\phi_1 - \cdots - c_{j-1,j}\phi_{j-1}) ,$$

yielding

(21) $$c_{ij} = (\phi_i, g_j) .$$

By (19),

(22) $$c_{1j} = d_1(g_1, g_j)$$

$$= d_1 a_{1j} , \qquad j = 2,3,\ldots,R .$$

By (20) and (21),

(23) $$c_{ij} = (g_j, d_i[g_i - c_{1i}\phi_1 - \cdots - c_{i-1,i}\phi_{i-1}])$$

$$= d_i[a_{ij} - c_{1i} c_{1j} - \cdots - c_{i-1,i}c_{i-1,j}] ,$$

$$j = 3,4,\ldots,R;\quad i = 1,2,\ldots,j-1 .$$

Further,

$$(\phi_1,\phi_1) = d_1^2 a_{11} = 1 ,$$

(24) $d_1 = a_{11}^{-\frac{1}{2}}$, and

$$(\phi_i,\phi_i) = 1 = d_i^2(g_i - c_{1i}\phi_1 - \cdots - c_{i-1,i}\phi_{i-1}, g_i - c_{1i}\phi_1 - \cdots - c_{i-1,i}\phi_{i-1})$$

$$d_i^{-2} = a_{ii} - 2(g_i, c_{1i}\phi_1 + \cdots + c_{i-1,i}\phi_{i-1}) + c_{1i}^2 + \cdots + c_{i-1,i}^2$$

(25) $$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} c_{ki}^2\right)^{-\frac{1}{2}}, \quad i=2,3,\ldots,R .$$

The set of functions defined by (19) - (20) and (22) - (25) are hence orthonormal as desired.

Since the set $\{\phi_i\}$ is orthonormal, the coefficients β_i which minimize

$$\frac{1}{M}\sum_{j=1}^{M}\left(h(y_j) - \sum_{i=1}^{R}\beta_i\phi_i(y_j)\right)^2$$

are

$$\beta_i = (h,\phi_i) , \qquad i=1,2,\ldots,R.$$

Using (19) and (20), we obtain

(26) $$\beta_1 = d_1 b_1$$

$$\beta_i = d_i(h, g_i - c_{1i}\phi_1 - \cdots - c_{i-1,i}\phi_{i-1})$$

(27) $$\beta_i = d_i [b_i - c_{1i}\beta_1 - \cdots - c_{i-1,i}\beta_{i-1}] ,$$

$$\text{for } i = 2,3,\ldots,R .$$

Since the functions ϕ_i are linear combinations of the g_i, $\Sigma \beta_i \phi_i$ constitutes a solution to the original problem (2). The α_i may be determined by setting

$$\Sigma \alpha_i g_i(x) = \Sigma \beta_i \phi_i(x)$$

and equating coefficients of g_i. By induction, one may show that equations (15) and (16) hold. Equations (8) - (16) constitute this constructive process. The reader may verify that the algorithm can be executed sequentially as listed.

Uniqueness of Solution

Clearly, solutions to (2) will not always be unique. If the sample points lie on a hypersurface of dimension less than R, infintely many solutions are possible.

On the other hand, the construction of the previous section indicates that a unique solution exists if the vectors $g_1, g_2, \ldots, g_R$ are linearly independent, since in that case d_i always exists. Since the $g_i(x)$ are linearly

independent functions of high dimension, the previous condition will be satisfied in practice "almost always".

Operation Count

The algorithm presented will often give significantly better results than solution of (3) directly [5] if operation count is a valid standard of comparison. Solution of (3) by Gaussian elimination requires

$$\frac{4R^3}{3} + R^2 - \frac{R}{3}$$

operations, counting only multiplications and divisions [3]. The algorithm presented requires

$$\frac{R^3}{6} + \frac{R^2}{2} + \frac{4}{3}R$$

operations (multiply and divide) and R square roots. Other than the square roots, direct solution requires

$$\frac{7}{6}R^3 + \frac{R^2}{2} - \frac{5}{3}R$$

more operations -- a significant difference.

Conclusion

The algorithm presented is more efficient than direct solution of the linear system derived from equation (2). It thus has clear advantages when the distribution function F is unknown. Storage of sample points is

unnecessary; working storage is limited to $\frac{R(R+3)}{2}$ words. A higher order approximation, if found necessary, may be derived with little recalculation.

If the distribution function is known, the usefulness of the algorithm will depend on the ease of generating random numbers with that distribution relative to the difficulty of direct solution or finding functions orthonormal with respect to the distribution function. Several of the other complications mentioned in the introduction may force recourse to the Monte Carlo approach.

This algorithm has proved useful in abstract pattern recognition where both $h(x)$ and $F(x)$ are unknown [4].

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